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Energy levels and radiative rates for transitions in Ni XIX*

K. M. Aggarwal and F. P. Keenan

Department of Physics and Astronomy, Queen's University, Belfast BT7 1NN, Northern Ireland, UK
e-mail: K.Aggarwal@qub.ac.uk

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ABSTRACT

Aims. In this paper we report calculations for energy levels and radiative rates for transitions in Ni XIX.
Methods. The General purpose Relativistic Atomic Structure Package (GRASP) has been adopted for the calculation of energy levels and radiative rates.
Results. Energies for the lowest 89 levels from the $(1s^2)\ 2s^22p^6$, $2s^22p^53\ell$, $2s2p^63\ell$, $2s^22p^54\ell$ and $2s2p^64\ell$ configurations of Ni XIX, are reported. Additionally, radiative rates, oscillator strengths, and line strengths are reported for all electric dipole (E1), magnetic dipole (M1), electric quadrupole (E2), and magnetic quadrupole (M2) transitions among these levels. Comparisons are made with the available results in the literature, and the accuracy of the present data is assessed. Finally, lifetimes for all excited levels are listed, and comparisons made with earlier available theoretical results.

Key words. atomic data – atomic processes

1. Introduction

Neon-like ions, particularly of the iron group of elements (namely Ti, Cr, Fe and Ni), are highly useful for the modelling and diagnostics of a variety of plasmas, such as astrophysical, fusion and laser generated plasmas. Many emission lines of nickel, including those from Ni XIX, have been observed in the sun – see, for example, Jupen (1984) and Feldman et al. (2000). Similarly many transitions, particularly within the $n = 3$ configurations, have been measured in laboratory plasmas by Feldman et al. (1967), Swartz et al. (1971), Boiko et al. (1977), Buchet et al. (1987) and Biémont et al. (2000). Therefore, atomic data (energy levels, radiative rates, collision strengths and excitation rates) for Ni XIX (and many other ions) are required for the modelling of plasmas, as well as diagnostics for their physical parameters, such as temperature and density. To fulfill this requirement, we have already reported results of energy levels and radiative rates for transitions in Ni XIII−XVI (Aggarwal et al. 2003) and Ni XVII (Aggarwal et al. 2007), and in this paper we present similar results for Ni XIX.

There have been a few calculations in the literature for Ni XIX, particularly by Loulergue & Nussbaumer (1975), Zhang et al. (1987), Zhang & Sampson (1989), and Hibbert et al. (1993). Loulergue & Nussbaumer reported values of energy levels and radiative rates (A-values). For the construction of wavefunctions, they included configuration interaction (CI) among 89 levels of the $(1s^2)\ 2s^22p^6$, $2s^22p^53\ell$, $2s2p^63\ell$, $2s^22p^54\ell$ and $2s2p^64\ell$ configurations, but reported energy levels and A-values only for *some* transitions among 57 levels. Furthermore, they calculated A-values for the electric dipole (E1) transitions alone, whereas in plasma modelling corresponding results for other types of transitions, namely magnetic dipole (M1), electric quadrupole (E2), and magnetic quadrupole (M2), may also be required. Similarly, Zhang et al. and Zhang & Sampson also calculated A-values, but for resonance E1 transitions alone. Finally, Hibbert et al. adopted the semi-relativistic CIV3 program (Hibbert 1975a) in which they included extensive CI with up to $n = 5$ orbitals. However, their calculations are restricted to E1 transitions among the lowest 37 levels of the $2s^22p^6$, $2s^22p^53\ell$ and $2s2p^63\ell$ configurations, whereas emission lines from the higher excited levels of the $n = 4$ and 5 configurations have already been measured (Swartz et al. 1971; Boiko et al. 1977; Biémont et al. 2000). Therefore, there is a clear need to extend the calculations to higher excited levels. Additionally, and more importantly, their energy levels, particularly for the levels of the $2s2p^63\ell$ configurations, differ by up to ~1.6 Ryd (2%) with those of Zhang & Sampson or the experimental values. Therefore, it has become essential to resolve this large discrepancy, apart from extending their calculations to higher excited levels, so that the results can be applied with confidence to the modelling of plasmas. Hence, in this paper we report energy levels and radiative rates for *all* transitions, and for all the four types mentioned above, because both of these requirements of having a complete set of data and for all types of transitions have recently been emphasized by Liedahl (2000), and demonstrated by Del Zanna et al. (2004).

In the present work, we mostly focus on the lowest 89 levels of the $2s^22p^6$, $2s^22p^53\ell$, $2s2p^63\ell$, $2s^22p^54\ell$ and $2s2p^64\ell$ configurations of Ni XIX, although calculations have been performed for a larger number of levels (157). Additionally, our approach is fully relativistic, as we employ the GRASP (General purpose Relativistic Atomic Structure Package) code of Dyall et al. (1989) to calculate radiative rates for the four types of transitions mentioned above. Finally, we also report lifetimes for all excited levels, and make comparisons with other available theoretical results.

2. Energy levels

The $2s^22p^6$, $2s^22p^53\ell$, $2s2p^63\ell$, $2s^22p^54\ell$ and $2s2p^64\ell$ configurations of Ni XIX give rise to 89 fine-structure levels, listed in

* Tables 3 and 4 are available only in electronic form at the CDS via anonymous ftp to cdsarc.u-strasbg.fr (130.79.128.5) or via http://cdsweb.u-strasbg.fr/cgi-bin/qcat?J/A+A/460/959

Table 1. Target levels of Ni XIX, their threshold energies (in Ryd) and lifetimes (τ in s). $a \pm b \equiv a \times 10^{\pm b}$.

Index	Configuration	Level	Expt.	LN	ZS	GRASP[a]	GRASP[b]	GRASP[c]	τ^d	τ^e
1	$2s^22p^6$	$^1S_0$	0.00000	0.000	0.0000	0.00000	0.00000	0.00000	.....	.....
2	$2s^22p^53s$	$^3P^o_2$	64.74789	64.651	64.7262	64.65407	64.59266	64.60110	2.108-06	2.125-06
3	$2s^22p^53s$	$^1P^o_1$	64.90591	66.026	66.1669	64.81635	64.75556	64.76398	6.851-13	6.886-13
4	$2s^22p^53s$	$^3P^o_0$	66.04590	65.925	66.0566	65.98467	65.89549	65.90393	2.205-05	2.205-05
5	$2s^22p^53s$	$^3P^o_1$	66.14067	64.813	64.8953	66.08407	65.99248	66.00089	8.639-13	8.687-13
6	$2s^22p^53p$	$^3S_1$	67.26964	66.892	67.2400	67.17989	67.11863	67.12572	2.319-10	2.327-10
7	$2s^22p^53p$	$^3D_2$	67.52411	67.165	67.5119	67.44378	67.38277	67.39132	1.456-10	1.458-10
8	$2s^22p^53p$	$^3D_3$	67.72295	67.368	67.7178	67.64860	67.57916	67.58763	1.262-10	1.263-10
9	$2s^22p^53p$	$^1P_1$	67.79872	68.395	67.7913	67.72326	67.65968	67.66821	1.376-10	1.375-10
10	$2s^22p^53p$	$^3P_2$	67.96467	67.608	67.9603	67.88865	67.82370	67.83239	9.417-11	9.424-11
11	$2s^22p^53p$	$^3P_0$	68.48787	68.138	68.5042	68.43553	68.36453	68.37167	8.498-11	8.480-11
12	$2s^22p^53p$	$^3D_1$	68.77114	68.720	68.7982	68.72702	68.63561	68.64413	1.757-10	1.756-10
13	$2s^22p^53p$	$^3P_1$	69.10029	67.442	69.1216	69.05203	68.95945	68.96780	1.119-10	1.119-10
14	$2s^22p^53p$	$^1D_2$	69.14025	69.040	69.1731	69.09959	69.00116	69.00972	1.049-10	1.051-10
15	$2s^22p^53p$	$^1S_0$	70.08373	69.883	70.2829	70.20187	70.13098	70.12033	2.980-11	3.014-11
16	$2s^22p^53d$	$^3P^o_0$	71.06029	70.530	71.0474	70.97559	70.91200	70.91987	7.318-11	7.335-11
17	$2s^22p^53d$	$^3P^o_1$	71.14900	70.626	71.1430	71.07218	71.00144	71.00934	6.579-12	6.564-12
18	$2s^22p^53d$	$^3P^o_2$	71.31366	70.804	71.3194	71.24548	71.16951	71.17763	7.524-11	7.536-11
19	$2s^22p^53d$	$^3F^o_4$	71.30920	70.816	71.3194	71.24872	71.16811	71.17517	7.866-11	7.887-11
20	$2s^22p^53d$	$^3F^o_3$	71.36068	70.860	71.3782	71.30334	71.22664	71.23402	6.555-11	6.565-11
21	$2s^22p^53d$	$^1D^o_2$	71.50804	72.206	71.5252	71.44977	71.37793	71.38611	6.317-11	6.320-11
22	$2s^22p^53d$	$^3D^o_3$	71.60408	71.120	71.6281	71.55273	71.47633	71.48470	6.954-11	6.953-11
23	$2s^22p^53d$	$^3D^o_1$	72.00285	71.550	72.0764	71.99795	71.91932	71.92557	8.806-14	8.804-14
24	$2s^22p^53d$	$^3F^o_2$	72.65054	72.122	72.7012	72.62254	72.51867	72.52627	6.377-11	6.386-11
25	$2s^22p^53d$	$^3D^o_2$	72.72649	71.008	72.7747	72.69682	72.59210	72.60051	7.158-11	7.161-11
26	$2s^22p^53d$	$^1F^o_3$	72.77962	72.269	72.8335	72.75651	72.64864	72.65641	7.330-11	7.335-11
27	$2s^22p^53d$	$^1P^o_1$	73.28227	72.874	73.4436	73.35168	73.24505	73.24640	2.832-14	2.874-14
28	$2s2p^63s$	$^3S_1$	76.16370	74.822	76.0309	75.99472	75.91019	75.91787	5.375-12	5.350-12
29	$2s2p^63s$	$^1S_0$	76.69223	75.364	76.5821	76.53857	76.45810	76.46122	7.771-12	7.776-12
30	$2s2p^63p$	$^3P^o_0$		77.249	78.7284	78.70060	78.62091	78.62883	5.817-12	5.818-12
31	$2s2p^63p$	$^3P^o_1$	78.56398	77.294	78.7725	78.74533	78.66211	78.67007	1.047-12	1.052-12
32	$2s2p^63p$	$^3P^o_2$		77.552	79.0371	79.00541	78.91529	78.92313	5.701-12	5.700-12
33	$2s2p^63p$	$^1P^o_1$	78.97314	77.707	79.1915	79.15871	79.06836	79.07669	1.987-13	1.994-13
34	$2s2p^63d$	$^3D_1$		80.828	82.4844	82.45243	82.35964	82.36300	6.964-12	7.091-12
35	$2s2p^63d$	$^3D_2$		80.852	82.4991	82.47276	82.37523	82.37867	6.825-12	6.941-12
36	$2s2p^63d$	$^3D_3$		80.894	82.5358	82.50711	82.40539	82.40894	6.703-12	6.810-12
37	$2s2p^63d$	$^1D_2$		81.316	82.9621	82.92779	82.82932	82.83494	5.643-12	5.691-12
38	$2s^22p^54s$	$^3P^o_2$		86.992	87.3576	87.25502	87.18001	87.18820	1.873-12	1.862-12
39	$2s^22p^54s$	$^1P^o_1$	87.34495	87.048	87.4090	87.30803	87.23366	87.24178	9.133-13	9.365-13
40	$2s^22p^54p$	$^3S_1$			88.4087	88.30838	88.23420	88.24100	1.976-12	1.953-12
41	$2s^22p^54p$	$^3D_2$			88.6365	88.37214	88.29789	88.30644	1.907-12	1.904-12
42	$2s^22p^54p$	$^3D_3$			88.5630	88.45761	88.37966	88.38816	2.024-12	2.007-12
43	$2s^22p^54p$	$^1P_1$			88.5851	88.48478	88.40888	88.41725	1.901-12	1.926-12
44	$2s^22p^54p$	$^3P_2$			89.9375	88.53920	88.46323	88.47188	2.059-12	2.060-12
45	$2s^22p^54s$	$^3P^o_0$		88.269	88.7027	88.59220	88.48770	88.49586	1.868-12	1.856-12
46	$2s^22p^54s$	$^3P^o_1$	88.62072	88.297	88.7321	88.61951	88.51422	88.52234	1.060-12	1.082-12
47	$2s^22p^54p$	$^3P_0$			88.9746	88.88798	88.81253	88.81156	2.125-12	2.182-12
48	$2s^22p^54p$	$^3D_1$			89.7905	89.68797	89.58303	89.59146	1.865-12	1.865-12
49	$2s^22p^54d$	$^3P^o_0$		89.265	89.8126	89.69949	89.62341	89.63083	1.128-12	1.115-12
50	$2s^22p^54d$	$^3P^o_1$	89.71424	89.306	89.8493	89.74025	89.66194	89.66951	1.040-12	1.032-12
51	$2s^22p^54d$	$^3F^o_4$	89.87827	89.360	89.9008	89.79252	89.71042	89.71858	1.126-12	1.118-12
52	$2s^22p^54d$	$^3P^o_2$		89.372	89.9155	89.80543	89.72552	89.73351	1.131-12	1.124-12
53	$2s^22p^54d$	$^3F^o_3$	91.15951	90.698	89.9155	89.81022	89.72977	89.73812	1.137-12	1.134-12
54	$2s^22p^54p$	$^3P_1$			89.9228	89.81331	89.70737	89.71520	2.041-12	2.034-12
55	$2s^22p^54p$	$^1D_2$			88.4748	89.83401	89.72619	89.73473	2.019-12	2.015-12
56	$2s^22p^54d$	$^1D^o_2$	91.18867	90.669	89.9669	89.86255	89.78376	89.79229	1.143-12	1.144-12
57	$2s^22p^54d$	$^3D^o_3$	89.89741	89.469	90.0037	89.89999	89.81961	89.82821	1.138-12	1.141-12
58	$2s^22p^54p$	$^1S_0$			90.1507	90.06286	89.96517	89.95715	2.058-12	2.138-12
59	$2s^22p^54d$	$^3D^o_1$	90.13342	89.703	90.2242	90.13488	90.05354	90.05585	9.439-14	9.926-14
60	$2s^22p^54f$	$^3D_1$			90.5696	90.45328	90.37202	90.38075	4.825-13	4.810-13
61	$2s^22p^54f$	$^1G_4$			90.5770	90.46263	90.37912	90.38694	5.116-13	5.110-13
62	$2s^22p^54f$	$^3G_5$			90.5843	90.46612	90.38262	90.39042	5.105-13	5.092-13
63	$2s^22p^54f$	$^3D_2$			90.5843	90.46836	90.38653	90.39524	4.901-13	4.896-13

Table 1. continued.

Index	Configuration	Level	Expt.	LN	ZS	GRASP[a]	GRASP[b]	GRASP[c]	τ^d	τ^e
64	$2s^22p^54f$	$^3F_3$			90.6137	90.50041	90.41809	90.42677	4.978-13	4.980-13
65	$2s^22p^54f$	$^1D_2$			90.6211	90.50525	90.42322	90.43188	5.119-13	5.146-13
66	$2s^22p^54f$	$^1F_3$			90.6211	90.50969	90.42724	90.43570	5.088-13	5.095-13
67	$2s^22p^54f$	$^3F_4$			90.6358	90.51836	90.43562	90.44406	5.108-13	5.118-13
68	$2s^22p^54d$	$^3F^\circ_2$		90.640	91.2459	91.13541	91.02549	91.03375	1.140-12	1.134-12
69	$2s^22p^54d$	$^3D^\circ_2$		89.428	91.2753	91.16235	91.05187	91.05988	1.132-12	1.127-12
70	$2s^22p^54d$	$^1F^\circ_3$		89.376	91.2973	91.18985	91.07845	91.08682	1.131-12	1.129-12
71	$2s^22p^54d$	$^1P^\circ_1$	91.33630	90.876	91.4664	91.36706	91.25686	91.25816	8.929-14	9.644-14
72	$2s^22p^54f$	$^3G_3$			91.9368	91.81666	91.70349	91.71148	5.093-13	5.088-13
73	$2s^22p^54f$	$^3G_4$			91.9515	91.82875	91.71542	91.72342	5.117-13	5.116-13
74	$2s^22p^54f$	$^3F_2$			91.9515	91.83513	91.72231	91.73097	5.062-13	5.077-13
75	$2s^22p^54f$	$^3D_3$			91.9588	91.83544	91.72243	91.73112	4.974-13	4.972-13
76	$2s2p^64s$	$^3S_1$			98.5079	98.44633	98.34835	98.36363	1.375-12	1.445-12
77	$2s2p^64s$	$^1S_0$			98.6917	98.63700	98.54064	98.54400	1.440-12	1.484-12
78	$2s2p^64p$	$^3P^\circ_0$		97.992	99.6031	99.54575	99.45014	99.47090	1.452-12	1.505-12
79	$2s2p^64p$	$^3P^\circ_1$	99.55593	98.008	99.6178	99.56155	99.46456	99.47209	7.905-13	3.700-13
80	$2s2p^64p$	$^3P^\circ_2$		98.115	99.7207	99.66750	99.56767	99.60480	1.516-12	1.661-12
81	$2s2p^64p$	$^1P^\circ_1$	99.70173	98.165	99.7721	99.71890	99.61892	99.59995	2.755-13	1.754-13
82	$2s2p^64d$	$^3D_1$			101.0217	100.96287	100.86169	100.87703	9.643-13	9.533-13
83	$2s2p^64d$	$^3D_2$			101.0290	100.97161	100.86875	100.88480	9.606-13	9.473-13
84	$2s2p^64d$	$^3D_3$			101.0511	100.98691	100.88248	100.89953	9.546-13	9.383-13
85	$2s2p^64d$	$^1D_2$			101.1907	101.13353	101.03066	101.04124	9.614-13	9.748-13
86	$2s2p^64f$	$^3F^\circ_2$			101.6979	101.62450	101.51947	101.53600	4.776-13	4.724-13
87	$2s2p^64f$	$^3F^\circ_3$			101.6979	101.62718	101.52125	101.54000	4.774-13	4.726-13
88	$2s2p^64f$	$^3F^\circ_4$			101.7053	101.63345	101.52723	101.54717	4.775-13	4.729-13
89	$2s2p^64f$	$^1F^\circ_3$			101.7200	101.64600	101.54040	101.55787	4.839-13	4.807-13

Expt.: NIST data from `http://www.physics.nist.gov/PhysRefData`
LN: Loulergue & Nussbaumer (1975).
ZS: Zhang & Sampson (1989).
[a] Present GRASP results for 89 levels *without* Breit and QED effects.
[b] Present GRASP results for 89 levels *with* Breit and QED effects.
[c] Present GRASP results for 157 levels *with* Breit and QED effects.
[d] Present GRASP results for 89 levels.
[e] Present GRASP results for 157 levels.

Table 1. A calculation performed with these 15 configurations is referred to as GRASP1. Since some levels of the $n = 5$ configurations interact with those of the $n = 4$ configurations, we have performed another calculation, referred to as GRASP2, in which we include a total of 157 levels. The additional 68 levels arise from the $2s^22p^55\ell$ and $2s2p^65\ell$ configurations. This will help us in assessing the accuracy of results for the lower levels.

Our calculated energies obtained from the GRASP code, from both the GRASP1 and GRASP2 calculations, are listed in Table 1 for the desired 89 levels. For our calculations, we have used the option of *extended average level* (EAL), in which a weighted (proportional to $2j + 1$) trace of the Hamiltonian matrix is minimized. This produces a compromise set of orbitals describing closely lying states with moderate accuracy. The calculations also include corrections from the Breit and QED effects. Also included in Table 1 are the experimental compilations of the National Institute of Standards and Technology (NIST), which are available at the website `http://physics.nist.gov/PhysRefData`, and the available theoretical results of Loulergue & Nussbaumer (1975) and Zhang & Sampson (1989).

Our energy levels from the GRASP1 and GRASP2 calculations agree closely (within 0.02 Ryd), except for the $2s2p^64p\ ^3P^\circ_2$ level (80), for which the difference is 0.04 Ryd. This indicates that the effect of the $n = 5$ configurations is negligible on the energy levels of the $n = 3$ and 4 configurations. This is mainly because the levels of the $n = 5$ configurations lie *above* the $2s^22p^54f\ ^3D_3$ (75) level, and hence a majority of these do not interact with the lower levels. Additionally, level orderings are the *same* in both calculations. However, some levels, such as: $(2s^22p^53p)\ ^3D_2$ and $^1D_2$ (7 and 14) and $(2s^22p^54p)\ ^3D_2$ and $^1D_2$ (41 and 55), are highly (or rather equally) mixed. Nevertheless, we have identified these levels on the basis of the strengths of their eigenvectors, in both calculations, and can state with confidence that there is no uncertainty in the designations of the levels in our listings in Table 1.

Our Breit and QED corrected energy levels agree with the experimental values within 0.25 Ryd (~0.3%) – see for example, levels 28 and 29. However, the differences for two levels, namely $(2s^22p^54d)\ ^3F^\circ_3$ and $^1D^\circ_2$ (53 and 56), are unexpectedly large, i.e. 1.4 Ryd or ~1.6%. As stated above, there is no ambiguity in our listings of the identification of the levels. However, a closer examination does reveal that these two levels are well mixed with two other levels, namely $^1F^\circ_3$ and $^3D^\circ_2$ (70 and 69), respectively. To be specific, the mixing coefficients of $^3F^\circ_3$ and $^1F^\circ_3$ are 0.760 and 0.582, respectively, and those of $^1D^\circ_2$ and $^3D^\circ_2$ are 0.726 and 0.459, respectively. Therefore, the identification of all these four levels is very clear. Nevertheless, if these two levels $^3F^\circ_3$ and $^1D^\circ_2$ are designated as $^1F^\circ_3$ and $^3D^\circ_2$, respectively, in the NIST data, then there is no discrepancy between theory and experiment. Finally, the energy levels of Zhang & Sampson (1989) also support our above conclusion, as their results agree with ours within 0.2 Ryd. However, they have probably misindentified the $(2s^22p^53s)\ ^1P^\circ_1$ and $^3P^\circ_1$ levels (3 and 5) in reverse

Table 2. Comparison of energy levels (in Ryd) of Ni XIX.

Index	Configuration	Level	Expt.	GRASP	FAC1	FAC2	FAC3	CIV3
1	$2s^22p^6$	$^1S_0$	0.00000	0.00000	0.0000	0.0000	0.0000	0.0000
2	$2s^22p^53s$	$^3P^o_2$	64.74789	64.59266	64.6260	64.6243	64.4843	64.7487
3	$2s^22p^53s$	$^1P^o_1$	64.90591	64.75556	64.7985	64.7975	64.6398	64.9061
4	$2s^22p^53s$	$^3P^o_0$	66.04590	65.89549	65.9271	65.9254	65.7771	66.0446
5	$2s^22p^53s$	$^3P^o_1$	66.14067	65.99248	66.0313	66.0302	65.8688	66.1407
6	$2s^22p^53p$	$^3S_1$	67.26964	67.11863	67.1474	67.1432	67.0258	67.2651
7	$2s^22p^53p$	$^3D_2$	67.52411	67.38277	67.4226	67.4217	67.2797	67.5369
8	$2s^22p^53p$	$^3D_3$	67.72295	67.57916	67.6142	67.6126	67.4797	67.7241
9	$2s^22p^53p$	$^1P_1$	67.79872	67.65968	67.6981	67.6972	67.5554	67.8000
10	$2s^22p^53p$	$^3P_2$	67.96467	67.82370	67.8663	67.8659	67.7191	67.9624
11	$2s^22p^53p$	$^3P_0$	68.48787	68.36453	68.4100	68.4089	68.2512	68.5097
12	$2s^22p^53p$	$^3D_1$	68.77114	68.63561	68.6713	68.6701	68.5236	68.7856
13	$2s^22p^53p$	$^3P_1$	69.10029	68.95945	68.9950	68.9937	68.8487	69.0956
14	$2s^22p^53p$	$^1D_2$	69.14025	69.00116	69.0392	69.0383	68.8875	69.1412
15	$2s^22p^53p$	$^1S_0$	70.08373	70.13098	70.2260	70.2142	69.9528	70.1169
16	$2s^22p^53d$	$^3P^o_0$	71.06029	70.91200	70.9373	70.9311	70.7882	71.0476
17	$2s^22p^53d$	$^3P^o_1$	71.14900	71.00144	71.0272	71.0213	70.8767	71.1404
18	$2s^22p^53d$	$^3P^o_2$	71.31366	71.16951	71.1944	71.1885	71.0422	71.3059
19	$2s^22p^53d$	$^3F^o_4$	71.30920	71.16811	71.1954	71.1904	71.0479	71.3149
20	$2s^22p^53d$	$^3F^o_3$	71.36068	71.22664	71.2481	71.2433	71.0934	71.3739
21	$2s^22p^53d$	$^1D^o_2$	71.50804	71.37793	71.3982	71.3949	71.2406	71.5139
22	$2s^22p^53d$	$^3D^o_3$	71.60408	71.47633	71.4981	71.4956	71.3360	71.6126
23	$2s^22p^53d$	$^3D^o_1$	72.00285	71.91932	71.9383	71.9363	71.7689	72.0459
24	$2s^22p^53d$	$^3F^o_2$	72.65054	72.51867	72.5450	72.5404	72.3843	72.6507
25	$2s^22p^53d$	$^3D^o_2$	72.72649	72.59210	72.6103	72.6068	72.4450	72.7172
26	$2s^22p^53d$	$^1F^o_3$	72.77962	72.64864	72.6662	72.6624	72.4993	72.7769
27	$2s^22p^53d$	$^1P^o_1$	73.28227	73.24505	73.2607	73.2589	73.0681	73.3565
28	$2s2p^63s$	$^3S_1$	76.16370	75.91019	75.9615	75.9601	75.8236	74.8222
29	$2s2p^63s$	$^1S_0$	76.69223	76.45810	76.5362	76.5328	76.3398	75.3098
30	$2s2p^63p$	$^3P^o_0$		78.62091	78.6761	78.6750	78.5453	77.2530
31	$2s2p^63p$	$^3P^o_1$	78.56398	78.66211	78.7185	78.7176	78.5857	77.2996
32	$2s2p^63p$	$^3P^o_2$		78.91529	78.9692	78.9679	78.8400	77.5506
33	$2s2p^63p$	$^1P^o_1$	78.97314	79.06836	79.1314	79.1314	78.9879	77.6960
34	$2s2p^63d$	$^3D_1$		82.35964	82.3940	82.3854	82.2644	80.8726
35	$2s2p^63d$	$^3D_2$		82.37523	82.4097	82.4011	82.2800	80.8917
36	$2s2p^63d$	$^3D_3$		82.40539	82.4397	82.4311	82.3103	80.9221
37	$2s2p^63d$	$^1D_2$		82.82932	82.8588	82.8563	82.7004	81.3372

Expt.: NIST data from `http://www.physics.nist.gov/PhysRefData`
GRASP: present GRASP results for 89 levels.
FAC1: Present FAC results for 89 levels.
FAC2: Present FAC results for 157 levels.
FAC3: Present FAC results for 3601 levels.
CIV3: Hibbert et al. (1993).

order, as seen in comparison with the experimental work or our calculations in Table 1. Additionally, the energy levels of the NIST compilations and the calculations of Zhang & Sampson agree comparatively better with our results performed *without* the inclusion of Breit and QED corrections, listed in Table 1 as GRASP^a, because Zhang & Sampson have omitted these in their calculations. The net effect of the Breit and QED corrections is to lower the energies by ∼0.11 Ryd.

The other results listed in Table 1 are from Loulergue & Nussbaumer (1975), who have included the same configurations as in our GRASP1 calculations, yet their energy levels differ by up to 1.8 Ryd (∼2.5%) with both experimental and other theoretical results, for many levels, such as: 13, 25, 28−37 and 69−81. Some of these differences are due to the misidentification of the levels – see, for example, levels 3/5 and 9/13, but for a majority of the levels (such as 78 and 81) the differences are in the calculational methods. Since their calculations were performed over three decades ago, with limited CI and including only the spin-orbit interaction term, it will be unfair to give too much emphasis to these differences in comparison to the present work. However, the energy levels of a more recent calculation by Hibbert et al. (1993) also agree with those of Loulergue & Nussbaumer, particularly for the levels of the $2s2p^63\ell$ configurations (28−37), and are in complete *disagreement* with the present or earlier calculations of Zhang & Sampson (1989) – see Table 2. Corresponding results from the experimental work are not available for all the levels, but are available for four levels (28, 29, 31 and 33), for which there is no agreement with the work of Loulergue & Nussbaumer or Hibbert et al. Since two independent calculations for 10 levels of the $2s2p^63\ell$ configurations differ substantially, by up to 1.8 Ryd (∼2%), with the present and earlier work of Zhang & Sampson, we discuss these further.

As stated earlier, Loulergue & Nussbaumer (1975) included the *same* basic configurations as included in our GRASP1 calculation or the one performed by Zhang & Sampson (1989), but Hibbert et al. (1993) included more extensive CI with up to $n = 5$ configurations as specified in their Table II. However, the similarity of results between the energy levels of

Loulergue & Nussbaumer and Hibbert et al. suggests that inclusion of extensive CI has no effect on the energy levels of the $n = 3$ (or even $n = 4$ as already discussed) configurations. Nevertheless, to confirm the accuracy of our results we have performed an exercise with the inclusion of extensive CI as included by Hibbert et al. To be specific, we have included 3601 levels arising from the $2s^22p^6$, $2s^22p^53\ell$, $2s^22p^54\ell$, $2s^22p^55\ell$, $2s2p^63\ell$, $2s2p^64\ell$, $2s2p^65\ell$, $2s2p^53\ell\ell'$, $2s^22p^43\ell\ell'$, $2s2p^53\ell4\ell$, $2s^22p^43\ell4\ell$, $2p^63\ell\ell'$, and $2p^63\ell4\ell$ configurations of Ni XIX. This calculation has been performed with the *Flexible Atomic Code* (FAC) of Gu (2003), which is available from the website `http://kipac-tree.stanford.edu/fac`. This is a fully relativistic code like GRASP, but is comparatively easier to run. Since results obtained from GRASP and FAC are generally in excellent agreement (see, for example, Aggarwal et al. 2007, for Mg-like ions or the present Table 2), our calculations from FAC enable us to assess the contribution of extensive CI in a fully relativistic work. We discuss these results below.

In Table 2, we list energy levels, for the lowest common 37 levels alone, from the experimental compilations of NIST along with a variety of the present calculations, from GRASP as well as FAC, and those of Hibbert et al. (1993). The corresponding energy levels of Zhang & Sampson (1989) and Loulergue & Nussbaumer (1975) are not included in this table, because they are similar to the present work and of Hibbert et al, respectively. Additionally, there are 3 calculations from FAC, namely FAC1 (89 levels from the $2s^22p^6$, $2s^22p^53\ell$, $2s2p^63\ell$, $2s^22p^54\ell$ and $2s2p^64\ell$ configurations, i.e. the same levels as included in GRASP1), FAC2 (157 levels, i.e. all those of FAC1 *plus* $2s^22p^55\ell$ and $2s2p^65\ell$, i.e. the same levels as included in GRASP2), and finally FAC3, which includes 3601 levels arising from the configurations specified above. Our energy levels from GRASP agree closely (within 0.1 Ryd) with those from FAC1 and FAC2, and the differences are only slightly higher (up to 0.18 Ryd or equivalently ≤0.25%) with those from FAC3. The CIV3 energy levels of Hibbert et al. for the lowest 27 levels are in excellent agreement with the experimental compilations of NIST. This is because their focus has been mainly on these levels. However, their energy values for the levels of the $2s2p^63\ell$ configurations (28−37) differ from any of our calculations or the compilations of NIST by up to 1.5 Ryd or equivalently ≤2%. The excellent agreement among a variety of our calculations, performed with differing amount of CI included and with two independent methods, confirms that the inclusion of extensive CI does not improve the energy levels of the $n = 3$ configurations of Ni XIX. Hence, we can state with confidence that the energy levels of Loulergue & Nussbaumer and Hibbert et al., although agreeing with each other, are not as accurate as reported by us or earlier by Zhang & Sampson, and are underestimated by up to 1.5 Ryd, especially for the levels of the $2s2p^63\ell$ configurations. This conclusion is also (partially) supported by the compilation of experimental energy levels by NIST.

3. Radiative rates

The absorption oscillator strength (f_{ij}) and radiative rate A_{ji} (in s^{-1}) for a transition $i \rightarrow j$ are related by the following expression:

$$f_{ij} = \frac{mc}{8\pi^2 e^2}\lambda_{ji}{}^2\frac{\omega_j}{\omega_i}A_{ji} = 1.49\times10^{-16}\lambda_{ji}^2(\omega_j/\omega_i)A_{ji} \quad (1)$$

where m and e are the electron mass and charge, respectively, c is the velocity of light, λ_{ji} is the transition energy/wavelength in Å, and ω_i and ω_j are the statistical weights of the lower (i) and upper (j) levels, respectively. Similarly, the oscillator strength f_{ij} (dimensionless) and the line strength S (in atomic unit, 1 au = 6.460×10^{-36} $cm^2\,esu^2$) are related by the following standard equations:

for the electric dipole (E1) transitions:

$$A_{ji} = \frac{2.0261\times10^{18}}{\omega_j\lambda_{ji}^3}S^{E1} \quad \text{and} \quad f_{ij} = \frac{303.75}{\lambda_{ji}\omega_i}S^{E1}, \quad (2)$$

for the magnetic dipole (M1) transitions:

$$A_{ji} = \frac{2.6974\times10^{13}}{\omega_j\lambda_{ji}^3}S^{M1} \quad \text{and} \quad f_{ij} = \frac{4.044\times10^{-3}}{\lambda_{ji}\omega_i}S^{M1}, \quad (3)$$

for the electric quadrupole (E2) transitions:

$$A_{ji} = \frac{1.1199\times10^{18}}{\omega_j\lambda_{ji}^5}S^{E2} \quad \text{and} \quad f_{ij} = \frac{167.89}{\lambda_{ji}^3\omega_i}S^{E2}, \quad (4)$$

and for the magnetic quadrupole (M2) transitions:

$$A_{ji} = \frac{1.4910\times10^{13}}{\omega_j\lambda_{ji}^5}S^{M2} \quad \text{and} \quad f_{ij} = \frac{2.236\times10^{-3}}{\lambda_{ji}^3\omega_i}S^{M2}. \quad (5)$$

In Table 3 we present transition energies (ΔE_{ij} in Å), radiative rates (A_{ji} in s^{-1}), oscillator strengths (f_{ij}, dimensionless), and line strengths (S in au), in length form only, for all 1210 electric dipole (E1) and 1468 electric quadrupole (E2) transitions among the 89 levels of Ni XIX. The indices used to represent the lower and upper levels of a transition have already been defined in Table 1. Similar results for 1172 magnetic dipole (M1) and 1505 magnetic quadrupole (M2) transitions are listed in Table 4.

Since the electric dipole (E1) transitions are comparatively more important, and most of the results available in the literature are confined to these transitions alone, we focus on the accuracy assessments of their f-values. In Table 5 we compare our results from the GRASP1, GRASP2 and FAC calculations with those of Hibbert et al. (1993) from the CIV3 code. The FAC calculations correspond to the FAC3 configurations described in Sect. 2, and the corresponding results of Zhang & Sampson (1989) are not included in this table, because their f-values are only for the resonance transitions, for which there is no discrepancy with our calculations. Furthermore, in this table we restrict the comparisons to transitions from the lowest 5 levels to levels up to 37. This comparison should give us sufficient information about the accuracy of our radiative rates.

Our f-values from the GRASP1, GRASP2 and FAC calculations generally agree within ∼10% for all the transitions listed in Table 5. This highly satisfactory agreement among the three calculations, with differing amount of CI included, clearly shows that the effect of extensive CI is negligible on the f-values. Similarly, the earlier obtained results of Hibbert et al. (1993) from the CIV3 code also generally agree within 10% for a majority of transitions. However, there are differences of up to 20% for some transitions, such as: 2−28, 3−28 and 4−28, whereas for the 5−29 ($2s^22p^53s\ {}^3P^\circ_1$−$2s2p^63s\ {}^1S_0$) transition their f-value is lower by 50% in comparison to all three other results listed in the table. Since all the transitions for which the f-values of Hibbert et al. differ substantially, including those which are not listed in Table 5, involve the higher excited levels of the $2s2p^63\ell$ configurations (28−37), the differences are clearly due to the inaccuracy in their determination of energy levels, as already discussed

Table 5. Comparison of oscillator strengths for some transitions of Ni XIX. ($a \pm b \equiv a \times 10^{\pm b}$).

Transition		GRASP1	GRASP2	FAC	CIV3
1	3	1.300-1	1.2931-1	1.252-1	1.254-1
1	5	9.927-2	9.8688-2	9.382-2	9.420-2
1	17	1.025-2	1.0273-2	9.979-3	1.130-2
1	23	8.188-1	8.1883-1	8.201-1	7.986-1
1	27	2.457-0	2.4206-0	2.287-0	2.300-0
1	31	4.709-2	4.6852-2	4.876-2	4.250-2
1	33	2.898-1	2.8881-1	2.894-1	2.767-1
2	6	4.957-2	4.9457-2	4.967-2	4.854-2
2	7	4.855-2	4.8515-2	4.733-2	4.742-2
2	8	1.548-1	1.5469-1	1.531-1	1.522-1
2	9	1.873-3	1.8944-3	1.662-3	1.940-3
2	10	6.557-2	6.5560-2	6.481-2	6.476-2
2	12	1.128-4	1.1365-4	1.142-4	1.200-4
2	13	3.868-3	3.8913-3	3.587-3	3.940-3
2	14	7.111-4	7.1384-4	6.739-4	7.400-4
2	28	6.660-2	6.6925-2	6.192-2	5.336-2
3	6	1.500-3	1.5137-3	1.415-3	1.567-3
3	7	8.620-2	8.6214-2	8.591-2	8.580-2
3	9	1.038-1	1.0380-1	1.026-1	1.015-1
3	10	9.025-2	9.0265-2	8.797-2	8.757-2
3	11	3.395-2	3.4100-2	3.356-2	3.440-2
3	12	3.303-4	3.3966-4	3.079-4	3.333-4
3	13	7.318-5	7.7306-5	6.551-5	6.667-5
3	14	8.679-4	8.5801-4	8.228-4	8.333-4
3	15	2.360-2	2.3411-2	2.247-2	2.157-2
3	28	2.867-2	2.8813-2	2.641-2	2.310-2
3	29	2.568-2	2.5681-2	2.409-2	1.890-2
4	6	1.157-3	1.1556-3	1.216-3	1.200-3
4	9	2.027-4	2.0351-4	1.915-4	2.000-4
4	12	1.130-1	1.1288-1	1.103-1	1.109-1
4	13	2.082-1	2.0805-1	2.069-1	2.048-1
4	28	6.083-2	6.1118-2	5.653-2	4.950-2
5	6	5.057-4	5.0582-4	5.352-4	5.000-4
5	9	3.113-5	2.9827-5	4.039-5	3.333-5
5	10	7.700-4	7.7368-4	7.448-4	7.333-4
5	11	8.211-3	8.1051-3	7.902-3	7.500-3
5	12	5.982-2	5.9843-2	5.948-2	5.920-1
5	13	3.826-2	3.8248-2	3.743-2	3.707-2
5	14	1.867-1	1.8663-1	1.841-1	1.833-1
5	15	4.149-2	4.1547-2	4.034-2	4.073-2
5	28	3.397-2	3.4138-2	3.184-2	2.757-2
5	29	1.645-2	1.6461-2	1.513-2	1.177-2
5	37	2.197-4	2.2982-4	2.493-4	2.000-4

GRASP1: present calculations from the GRASP code with 89 levels.
GRASP2: present calculations from the GRASP code with 157 levels.
FAC: present calculations from the FAC code with 3601 levels.
CIV3: calculations of Hibbert et al. (1993) from the CIV3 code.

in Sect. 2. Therefore, there is no discrepancy with the reported f-values of Hibbert et al. for transitions involving lower levels up to 27, but their results for those transitions which involve the higher excited levels of the $2s2p^6 3\ell$ configurations are not very accurate, and differ from our calculations by up to 50%. However, before forming conclusions on the accuracy of our results, we make some other assessments below for a larger number of transitions, because the transitions in Table 5 represent only a fraction of a total of 1210.

A general criterion to assess the accuracy of the A- or f-values is to compare their length and velocity forms. Before we discuss these we would like to remind readers that such comparisons are desirable, but are *not* a fully sufficient tests to assess the accuracies (Hibbert 1975b), as different calculations (or combinations of configurations) may give comparable f-values in the two forms, but entirely different results in magnitude – see Aggarwal et al. (2007) for further details and comparisons. Nevertheless, we discuss the two forms below in order to make some assessment about the accuracy of the results.

Among the stronger transitions (i.e. $f \geq 0.01$), the length and velocity forms agree to better than 20% for all transitions, except for 11−27 ($2s^2 2p^5 3p\ ^3P_0 - 2s^2 2p^5 3d\ ^1P^\circ_1$; $f_L = 0.017$) for which $f_L/f_V = 1.5$. This is highly satisfactory and in a way confirms the accuracy of our calculations. However, differences between the two forms for weaker transitions ($f < 0.01$) are up to several orders of magnitude, particularly for those whose f-values are $\sim 10^{-5}$ or smaller. Examples of such transitions are: 7−80 ($f = 1.3 \times 10^{-5}$), 14−81 ($f = 1.5 \times 10^{-5}$) and 52−55 ($f = 9.2 \times 10^{-8}$). Such large differences for weak transitions are very common, and mainly arise from the cancellation effect of the mixing coefficients and/or the inclusion/exclusion of large CI. Although the f- or A-values for such transitions may be required in modelling work, their contribution is much less important in comparison to those from the stronger transitions. Therefore, a larger variation in their values among different calculations, and/or between their f_L and f_V values, do not affect the overall accuracy of a calculation. To conclude, based on a satisfactory agreement between the two forms, we may state that the accuracy of our listed A-values is better than 20% for all *strong* transitions.

4. Lifetimes

The lifetime τ for a level j is defined as follows:

$$\tau_j = \frac{1}{\sum_i A_{ji}}. \quad (6)$$

Since this is a measurable parameter, it provides a check on the accuracy of the calculations. In Table 1 we list our calculated lifetimes, from both the GRASP1 and GRASP2 calculations, which *include* the contributions from all four types of transitions, i.e. E1, E2, M1 and M2. These results are helpful for comparisons with theory or experiments. The two sets of lifetimes agree closely, except for two levels, namely $(2s2p^6 4p)\ ^3P^\circ_1$ and $^1P^\circ_1$ (79 and 81), for which the differences are up to a factor of two. However, the lifetimes for both of these levels are very small, i.e. $\tau \sim 10^{-13}$ s.

To our knowledge, no measurements of lifetimes are available for levels of Ni XIX, but Hibbert et al. (1993) have reported calculations for some levels of the $2s^2 2p^5 3\ell$ configurations. We compare their results with our calculations in Table 6. In general, agreement between the two calculations is within 10%, which is highly satisfactory. However, the difference for the $2s^2 2p^5 3p\ ^1D_2$ level (14) is ∼20%, which is due to the fact that Hibbert et al. have performed calculations for the E1 transitions alone, whereas we have also included the contributions of the E2, M1 and M2 transitions. For most of the levels listed in Table 6 the contributions of the E1 transitions are *dominant*, but for the $^1D_2$ level, the E2 transition 1−14 makes a significant contribution, as its A-value is 1.20×10^9 s^{-1} while that of the dominant 5−14 E1 transition is 8.14×10^9 s^{-1}. To conclude, we may state that there is no discrepancy for the lifetimes between two independent calculations, because for the lowest 27 levels there is no discrepancy for the A-values either.

5. Conclusions

In the present work, results for energy levels, radiative rates, oscillator strengths, and line strengths for transitions among the

Table 6. Comparison of lifetimes (τ in ns) for some levels of Ni XIX. $a \pm b \equiv a \times 10^{\pm b}$.

Index	Level	Present Calculations	Hibbert et al. (1993)
6	$2s^2 2p^5 3p\ ^3S_1$	2.319-1	2.38-1
7	$2s^2 2p^5 3p\ ^3D_2$	1.456-1	1.72-1
8	$2s^2 2p^5 3p\ ^3D_3$	1.262-1	1.29-1
9	$2s^2 2p^5 3p\ ^1P_1$	1.376-1	1.41-1
10	$2s^2 2p^5 3p\ ^3P_2$	9.417-2	1.07-1
11	$2s^2 2p^5 3p\ ^3P_0$	8.498-2	8.49-2
12	$2s^2 2p^5 3p\ ^3D_1$	1.757-1	1.78-1
13	$2s^2 2p^5 3p\ ^3P_1$	1.119-1	1.15-1
14	$2s^2 2p^5 3p\ ^1D_2$	1.049-1	1.23-1
15	$2s^2 2p^5 3p\ ^1S_0$	2.980-2	3.37-2
3	$2s^2 2p^5 3s\ ^1P^\circ_1$	6.851-4	7.07-4
5	$2s^2 2p^5 3s\ ^3P^\circ_1$	8.639-4	9.07-4
16	$2s^2 2p^5 3d\ ^3P^\circ_0$	7.318-2	7.57-2
17	$2s^2 2p^5 3d\ ^3P^\circ_1$	6.579-3	6.03-3
18	$2s^2 2p^5 3d\ ^3P^\circ_2$	7.524-2	7.76-2
19	$2s^2 2p^5 3d\ ^3F^\circ_4$	7.866-2	8.00-2
20	$2s^2 2p^5 3d\ ^3F^\circ_3$	6.555-2	6.69-2
21	$2s^2 2p^5 3d\ ^1D^\circ_2$	6.317-2	6.46-2
22	$2s^2 2p^5 3d\ ^3D^\circ_3$	6.954-2	7.08-2
23	$2s^2 2p^5 3d\ ^3D^\circ_1$	8.806-5	9.00-5
24	$2s^2 2p^5 3d\ ^3F^\circ_2$	6.377-2	6.58-2
25	$2s^2 2p^5 3d\ ^3D^\circ_2$	7.158-2	7.35-2
26	$2s^2 2p^5 3d\ ^1F^\circ_3$	7.330-2	7.52-2
27	$2s^2 2p^5 3d\ ^1P^\circ_1$	2.832-5	3.02-5

89 levels of Ni XIX have been presented for *all* permissible transitions. These results cover a substantially larger number of transitions than previously available in the literature. Additionally, results for radiative rates have been presented for four types of transitions, namely E1, E2, M1 and M2. A complete set of results are likely to be useful for the modelling of a variety of plasmas. Furthermore, calculations for A-values have also been performed for a larger number of transitions among 157 levels, which include additional 68 levels of the $2s^2 2p^5 5\ell$ and $2s2p^6 5\ell$ configurations. This entire set of data for 3401 E1, 4439 E2, 3334 M1 and 4503 M2 transitions can be obtained in electronic form on request from KMA (K.Aggarwal@qub.ac.uk).

Based on the comparison made among a variety of calculations, and adopting both the GRASP and FAC codes with differing amount of CI, as well as with the available compiled experimental and other theoretical results, our energy levels are assessed to be accurate to better than 1%. We have also demonstrated that the earlier available energy levels of Loulergue & Nussbaumer (1975) and Hibbert et al. (1993) are underestimated by up to 1.5 Ryd for several levels, particularly the higher ones. Similarly, based on the comparison made between the length and velocity forms of the oscillator strengths, as well as among a variety of calculations with differing amount of CI included, we assess that our radiative rates are accurate to better than 20% for all strong transitions. However, for weaker transitions the A- or f-values are less accurate.

Lifetimes for all excited levels of Ni XIX are listed, but comparison with the corresponding available results has been possible for only a few levels, for which there are no discrepancies.

To assess the accuracy of our presented results, we also performed a larger calculation (with up to 3601 levels) from FAC, which included more elaborate CI than in our GRASP calculations. However, the energy levels and A-values from GRASP have been preferred, mainly for two reasons. Firstly, as discussed in Sects. 2 and 3, the results obtained from the simpler GRASP calculations are of comparable accuracy with those from the larger calculation. Secondly, and more importantly, a collisional calculation for 3601 levels is currently not feasible with the resources available to us. Therefore, our calculations for a more important parameter namely collision strength, and subsequently for excitation rate coefficient, are in progress only for the lowest 89 levels of Ni XIX. Thus the presently reported results will be consistent with the collisional work. Nevertheless, energy levels and radiative rates for all the 3601 levels can be obtained in electronic form on request from KMA (K.Aggarwal@qub.ac.uk).

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